

Isotopic chains around oxygen from evolved chiral two- and three-nucleon interactions

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(Dated: March 21, 2013)

We extend the formalism of self-consistent Green's function theory to include three-body interactions and apply it to isotopic chains around oxygen for the first time. The third-order algebraic diagrammatic construction [ADC(3)] equations for two-body Hamiltonians can be exploited upon defining system-dependent one- and two-body interactions coming from the three-body force, and correspondingly dropping interaction reducible diagrams. This goes beyond the standard normal ordering truncations recently used in ab-initio studies. The Koltun sum rule for the total binding energy acquires a correction due to the added three-body interaction. This formalism is then applied to study chiral two-nucleon (2N) and three-nucleon forces (3NF) evolved to low momentum cutoffs. We find that these interactions reproduce the binding energies of nitrogen, oxygen and fluorine isotopes to great accuracy, providing clear indication of the predictive power of this approach. All three neutron driplines are correctly predicted when full 3NF are included. The formalism introduced also allows to calculate form factors for nucleon transfer on doubly magic systems.

PACS numbers: 21.10.-k, 21.30.Fe, 21.60.De

Introduction. - The ultimate goal of ab-initio nuclear theory is to achieve accurate predictions of nuclear properties that are consistent with the underlying theory of QCD and are parameter free as much as possible. Advancing on this problem is presently of primary importance in the mid mass region of the nuclear chart, in response to significant advances in the discovery of new nuclides at radioactive isotope facilities [1]. Moreover, parameter free predictions would help reducing uncertainties in our knowledge of dripline isotopes that are currently beyond experimental reach [2]. The requirement of accuracy poses strong requirements on both the knowledge of the nuclear interaction and the many-body techniques used in the calculations.

Breakthroughs over the last decade were possible due to the introduction of many-body methods that scale gently with increasing particle number and therefore can reach systems well above the p shell. Self consistent Green's function theory (SCGF) [3, 4], coupled cluster (CC) [5–7] and in-medium similarity renormalization group (IM-SRG) [8, 9] have been employed in ab-initio calculations of doubly closed shell nuclei with masses up to $A \sim 60$. For open-shells, semi-magic isotopes can be calculated by breaking particle conservation symmetry and reformulating theories in terms of Hartree-Fock Bogolioubov reference states as done in Gorkov theory [10] and in IM-SRG. Calculations based on IM-SRG have been performed for ground state energies [9]. On the other hand, the state-of-the-art SCGF theory not only can be extended to open shells [11] but it gives access to a wealth of nuclear structure information. This includes the addition or removal of one or two nucleons to/from the calculated ground states [12, 13] and direct link to microscopic optical potentials [14].

In this Letter, we extend the scope of SCGF to include three-nucleon forces (3NFs) in finite nuclei. We define density dependent one- and two-body forces derived from the 3NF part of the hamiltonian and work out the first order correction to the Koltun sum rule to obtain binding energies. The method

is applied to the isotopic chains of oxygen, nitrogen and fluorine, as well as spectra of single-neutron states in the sd shell. This opens the possibility of probing modern realistic nuclear interactions on a wide range of experimental data, including excitation spectra, the evolution of shell closures, and the position of driplines.

Formalism. We employ Green's function (or propagator) theory, where the object of interest is the single particle propagator [15].

$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\omega - \varepsilon_n^{A+1} + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\omega - \varepsilon_k^{A-1} - i\eta}, \quad (1)$$

where greek indices α, β, \dots , label a complete orthonormal basis set and $\varepsilon_n^{A+1} \equiv (E_n^{A+1} - E_0^A)$ and $\varepsilon_k^{A-1} \equiv (E_0^A - E_k^{A-1})$ are the nucleon addition and separation energies, respectively. In Eq. (1), $|\Psi_n^{A+1}\rangle$, $|\Psi_k^{A-1}\rangle$ are the eigenstates and E_n^{A+1} , E_k^{A-1} are the eigenenergies of the $(A \pm 1)$ -nucleon system. Hence, $g_{\alpha\beta}(\omega)$ describes the exact propagation of a single-nucleon or hole excitation through the system. From Eq. (1) we also extract the one-body reduced density matrix,

$$\rho_{\alpha\beta} = \langle \Psi_0^A | c_\beta^\dagger c_\alpha | \Psi_0^A \rangle = \int_{C \uparrow} d\omega g_{\alpha\beta}(\omega), \quad (2)$$

where the integration contour $C \uparrow$ is taken on the upper half of the imaginary plane.

We start our calculations with the intrinsic Hamiltonian $H(A) = H - T_{c.m.}(A) = U(A) + V(A) + W$ in which the kinetic energy of the center of mass (c.o.m.) has been subtracted and we put in evidence the dependence on the number of nucleons A . The terms U , V and W collect all the one-, two- and three-nucleon contributions, respectively. Based on this, we define system dependent one- and two-body effective interactions obtained by contraction with the correlated density

matrix, Eq. (1),

$$\tilde{U}_{\alpha\beta} = U_{\alpha\beta} + V_{\alpha\gamma,\beta\delta}\rho_{\delta\gamma} + \frac{1}{2}W_{\alpha\gamma\delta,\beta\mu\nu}\rho_{\mu\gamma}\rho_{\nu\delta}, \quad (3)$$

$$\tilde{V}_{\alpha\beta,\gamma\delta} = V_{\alpha\beta,\gamma\delta} + W_{\alpha\beta\mu,\gamma\delta\nu}\rho_{\nu\mu}. \quad (4)$$

where all matrix elements are properly antisymmetrized and summation over repeated indices are implied here and in the following. The resulting Hamiltonian, $\tilde{H} = \tilde{U} + \tilde{V} + W$, can be proved to lead to the same Green function (1) for the original hamiltonian with the caveat that only *interaction irreducible* must be retained in their diagrammatic expansion [16]¹. Equations (3) and (4) generalize the idea of normal ordering of the Hamiltonian to fully correlated densities. In the following we retain only the \tilde{U} and \tilde{V} terms and discard diagrams with explicit interaction irreducible 3NF terms. This approximation has been proven to be negligible for the present hamiltonians in [17, 18]². The single-particle propagator $g_{\alpha\beta}(\omega)$ can then be calculated for finite closed-shell nuclei by exploiting the effective one- and two- body interactions with the already available two-body formalism.

We first solve the spherical Hartree-Fock (HF) equations for the full Hamiltonian within the given model space. The resulting propagator, $g_{\alpha\beta}^{HF}(\omega)$, is then used as a reference state to calculate the energy-dependent contribution to the self-energy. We employ the third-order algebraic diagrammatic construction [ADC(3)] method [19, 20] and write the self-energy as

$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{\infty} + \Sigma'_{\alpha\beta}(\omega) \quad (5)$$

$$= \tilde{U}_{\alpha\beta} + C_{an} \left[\frac{1}{\omega - M} \right]_{nn'} C_{n'\beta}^\dagger + D_{ak} \left[\frac{1}{\omega - N} \right]_{kk'} D_{k'\beta}^\dagger,$$

where \mathbf{M} (\mathbf{N}) are interaction matrices in the $2h1p$ ($2p1h$) space and \mathbf{C} (\mathbf{D}) are the corresponding coupling strength to the single particle states. In the ADC(3), these matrices are constructed to guarantee that all diagrams up to third order are included in Eq.(5). We note that the ADC(n) approach defines a hierarchy of truncation schemes for increasing order n to guide systematic improvements of the method. The correlated propagator $g_{\alpha\beta}(\omega)$ is finally obtained by solving the Dyson equation,

$$g_{\alpha\beta}(\omega) = g_{\alpha\beta}^{HF}(\omega) + g_{\alpha\gamma}^{HF}(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega), \quad (6)$$

which is diagonalized using a Lanczos algorithm as explained extensively in [21, 22]. Note that we employ the *sc0* approximation of Refs. [11, 22] in which only the $\Sigma'_{\alpha\beta}(\omega)$ contribution of Eq. (5) depends on the reference states $g_{\alpha\beta}^{HF}(\omega)$. This implies the iterative solutions of Eq. (6) to evaluate $\Sigma_{\alpha\beta}^{\infty} = \tilde{U}_{\alpha\beta}$ in terms of the final correlated density matrix, Eq. (3).

In presence of 3NFs, the ground state energy can still be inferred from the Koltun sum rule (SR) that now acquires a correction:

$$E_0^A = \sum_{\alpha\beta} \frac{1}{4\pi i} \int_{C^\dagger} d\omega \left[U_{\alpha\beta} + \omega \delta_{\alpha\beta} \right] g_{\beta\alpha}(\omega) - \frac{1}{2} \langle \Psi_0^A | W | \Psi_0^A \rangle. \quad (7)$$

Eq. (7) is still an exact equation. However, it requires to evaluate the expectation value of the 3NF part of the hamiltonian $\langle \Psi_0^A | W | \Psi_0^A \rangle$, with an accuracy comparable to the many-body approximation in use. We calculate this correction at first order in W using fully correlated propagators,

$$\langle W^{3p} \rangle = \frac{1}{6} W_{\alpha\beta\gamma,\mu\nu\xi} \rho_{\mu\alpha} \rho_{\nu\beta} \rho_{\xi\gamma} \quad (8)$$

that implicitly includes relevant higher order terms from standard many-body perturbation theory. We found that it is mandatory to use the fully dressed propagators, i.e. solutions of the Eq. (6), but this is sufficient to account for all relevant contributions. The next order correction is given by

$$\langle W^{TDA} \rangle = \frac{1}{4} W_{\alpha\beta\gamma,\mu\nu\xi} \rho_{\mu\alpha} \Delta\Gamma_{\nu\xi,\beta\gamma}. \quad (9)$$

where $\Delta\Gamma$ is the two-body density matrix after subtraction of the zeroth-order contribution coming from two *fully correlated* but *non-interacting* nucleons, to avoid double counting Eq. (8). We estimated this using in Tamn-Dancoff approximation (TDA) [23] and found its contribution to be small compared to our estimated errors, as discussed below.

The binding energy and spectra of neighboring even-odd isotopes are extracted from the poles of propagator (1), however this requires a proper correction to account for the variation in the kinetic energy of the c.o.m. motion with changing A . To extract the energy of a system with mass $A \pm 1$, we recalculate $g_{\alpha\beta}(\omega)$ for the doubly closed-subshell A -nucleon system but with a $\tilde{H}(A \pm 1)$ corrected hamiltonian. We then obtain:

$$E^{A\pm 1} = \pm \varepsilon_0^{A\pm 1} [\tilde{H}(A \pm 1)] + E_0^A [\tilde{H}(A \pm 1)], \quad (10)$$

where we made explicit the dependence on c.o.m. correction for the Hamiltonian and $E_0^A [\tilde{H}(A \pm 1)]$ is obtained from the corrected Koltun SR.

Results. We perform calculations using chiral effective field theory (EFT) two-nucleon (2N) and 3NFs evolved to low momentum scales by using free-space similarity renormalization group (SRG) [24, 25]. The original 2N interaction is N³LO with cutoff $\Lambda_{2N}=500$ MeV [26, 27] while for the 3NF we chose a N²LO in a local form [28] with a reduced cutoff of $\Lambda_{3N}=400$ MeV and low-energy constants $c_D=-0.2$ and $c_E=0.098$ refitted to reproduce the ⁴He binding energies, as discussed in Ref. [29]. The SRG evolution on the sole 2N-N³LO interaction already generates 3N interactions, which we will refer hereafter to as “induced” 3NFs. When the pre-existing 3N-N²LO interaction is included in the SRG evolved interaction will be referred to as “full” 3NFs. The two-pion

¹ A diagram is said to be *interaction reducible* if it can be factorized in two lower-order diagrams by cutting an interaction vertex or, equivalently, if there exists a group of lines (interacting or not) that leave an interaction vertex and eventually all return to it.

² This would be the analogous to the NO2B approximation of Ref. [18] but, here, not tight to the choice of any reference state.

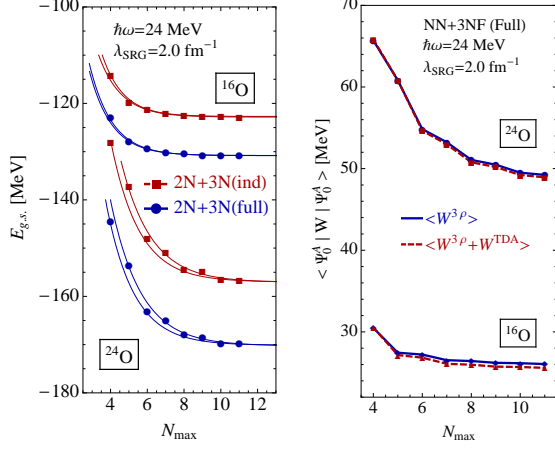


FIG. 1. (Color online) Convergence of ^{16}O and ^{24}O as a function of increasing size of the model space for $\hbar\omega=24$ MeV and $\lambda_{\text{SRG}}=2.0$ fm $^{-1}$. *Left*: Binding energies from the corrected Koltun sum rule, Eq. (7), as obtained from the induced and full interactions. *Right*: Expectation value $\langle \Psi_0^A | W | \Psi_0^A \rangle$ obtained at first order only, Eq. (8), (full lines) and with correction from two-body TDA ladders, Eq. (9) (dashed lines).

exchange diagrams that incorporate physics from the Fujita-Miyazawa 3NF appear in the chiral 3N- N^2LO force and therefore their effects are incorporated only in the full Hamiltonian. Calculations were performed in model spaces up to 12 harmonic oscillator shells [$N_{\max} \equiv \max(2n + l) = 11$], including all 2N matrix elements and limiting 3NF ones to configurations with $N_1 + N_2 + N_3 \leq N_{3\text{NF},\max} = 14$. Except when indicated, a SRG cutoff $\lambda=2.0$ fm $^{-1}$ and harmonic oscillator frequency $\hbar\omega=24$ MeV were used.

Figure 1 shows the convergence pattern of the total binding energy of ^{16}O and ^{24}O as a function of the model space size. The convergence is optimized by the choice of the chosen oscillator frequency which is close to the minimum of the $\hbar\omega$ dependence for the present interaction [9]. The staggering between adjacent results is due to the particular truncation of 3NF matrix elements and the alternate parities of harmonic oscillator shells. Separate exponential fits to the calculated ^{24}O energies, for N_{\max} either even or odd, differ by 100 keV and are within 600 keV of the $N_{\max}=11$ result, with an overall error of 0.5% of the total binding energy. The right panel of Fig. 1 demonstrates the similar convergence of the $\langle \Psi_0^A | W | \Psi_0^A \rangle$ expectation values. The contribution of $\langle W^{\text{TDA}} \rangle$, Eq. (9), is never bigger than 300 keV and represent a small correction to $\langle W \rangle$. A proper study of the contributions to $\langle W \rangle$ will be addressed in a forthcoming publication. For the present purposes, we sum the above uncertainties to make a conservative estimate for our convergence error of 1% for the calculated total binding energies.

The differences between calculated binding energies the experiment, are demonstrated in Fig. 2 for three different com-

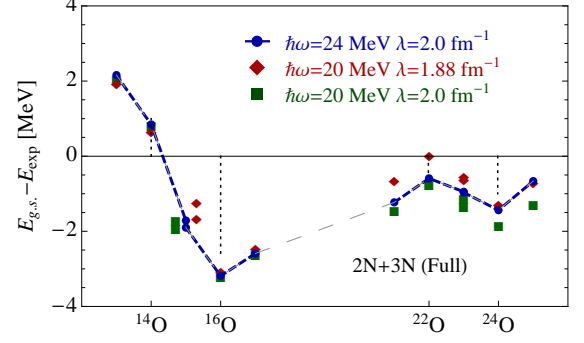


FIG. 2. (Color online) Differences between calculated and experimental ground state energies of oxygen isotopes for the full interaction with different values of $\hbar\omega$ and λ_{SRG} .

binations of the $\hbar\omega$ and λ_{SRG} . Changes with the variation of these parameters are rather small and increase only slightly going to larger masses. For ^{24}O we find about 450 keV variations for $\hbar\omega$ between 20 and 24 MeV. This is 0.3% of the total energy, which is well within our estimated error from convergence. Changes from λ_{SRG} in the range 1.88-2.0 fm $^{-1}$ are also small and in agreement with the 1% estimated from larger ranges of the cutoff [9].

From previous studies based on the ADC(3) method, we expect accuracy of the many-body truncation scheme of about 1% [30, 31]. The extrapolated ^{16}O ground state (Fig. 1) is over bound at -130.8(1) MeV but in close agreement with the -130.5(1) MeV obtained from IM-SRG [9], giving further confirmation of the accuracy achieved by different many-body methods. Binding energies of ^{15}O and ^{23}O can be obtained in two different ways, from either neutron addition or removal on neighboring sub-shell closures. Results differ by at most 400 keV, again within the estimated uncertainty of our many-body truncation scheme. The correction (10) is crucial to obtain this agreement. For $\hbar\omega=24$ MeV and $\lambda_{\text{SRG}}=2.0$ fm $^{-1}$, the discrepancy in ^{15}O (^{23}O) is 1.65 MeV (1.05 MeV) when neglecting the changes in kinetic energy of the c.o.m. but it reduces to only 190 keV (20 keV) when this is accounted for. This gives us confidence on the procedure to separate the effects of the center of mass motion and an additional confirmation of the quality of the method.

Fig. 2 also gives a first remarkable demonstration of the predictive power of chiral 2N+3N interactions: accounting for the precision of our many-body approach and dependence over larger ranges of cutoffs we expect an accuracy of $\approx 3\%$ on binding energies and all calculated values agree with the experiment within this limits. Note that the interaction employed were only constrained by 2N and $^3\text{H}/^4\text{He}$ data.

Figure 3 collects our results for the oxygen isotopic chain, as calculated for $\hbar\omega=24$ MeV and $\lambda_{\text{SRG}}=2.0$ fm $^{-1}$. The top panel demonstrates the evolution of neutron single particle spectrum in the sd shell. Induced 3NFs reproduce the overall trend but predict a bound $d_{3/2}$ orbit for the neutron rich isotopes. The main consequence of adding pre-existing 3NFs—

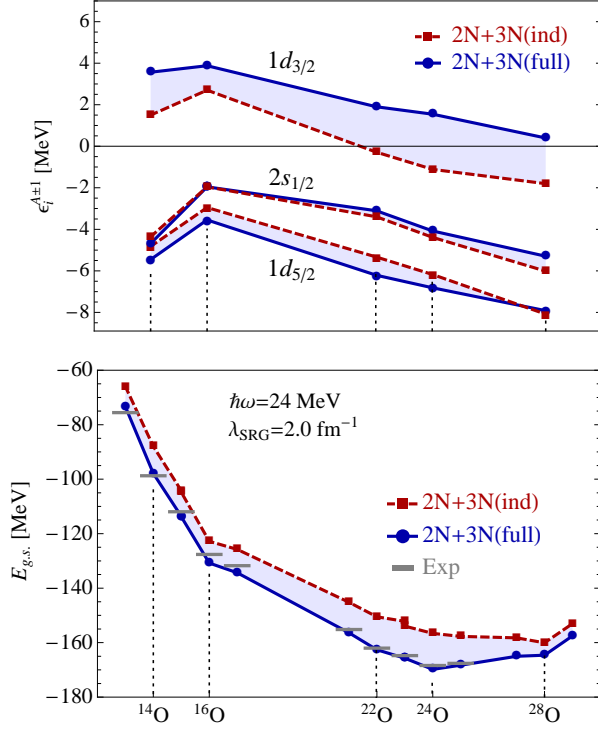


FIG. 3. (Color online) *Top*. Evolution of single-particle energies for neutron addition and removal around sub-shell closures of oxygen isotopes. *Bottom*. Binding energies obtained from the Koltun SR and the poles of propagator (1), compared to experiment (bars) [32, 33]. All points are corrected for the kinetic energy of the c.o.m. motion. For all lines, red squares (blue dots) refer to induced (full) 3NFs.

the full Hamiltonian—is to raise this last orbit above the continuum threshold and confirms the increasing repulsive effects of the two-pion exchange Fujita-Miyazawa interaction on this orbits, as the neutron sd shell is filled [34]. Instead, the $d_{5/2}$ quasiparticle states are lowered by about 1 MeV on average, providing extra binding through the Koltun SR formula (7). The consequences of this trends are demonstrated by the calculated ground state energies shown in the bottom panel: the induced hamiltonian systematically under binds the whole isotopic chain, and confirms earlier predictions based solely on the original 2N-N3LO interaction [35]. The dripline is also erroneously placed at ^{28}O because of the lack of repulsion in the $d_{3/2}$ orbit. On the other hand, contributions from pre-existing 3NFs are substantial and increase with the mass number up to ^{24}O , when the unbound $d_{3/2}$ orbit starts being filled. As a result, the full Hamiltonian nicely reproduces both the experimental ground state energies and the observed dripline at ^{24}O [36]. Our result suggest a ground state resonance for ^{28}O unbound by 5.2 MeV with respect to ^{24}O . However this estimate is likely to be affected the presence of the continuum which is important for this nucleus but neglected in the present work.

The same effects are demonstrated in Fig. 4 for the semi-

magic odd-even isotopes of nitrogen and fluorine. Induced 3NF forces consistently under bind these isotopes and even predict a ^{27}N close in energy to ^{23}N . This is fully corrected by full 3NFs that strongly binds ^{23}N with respect to ^{27}N , in accordance with the experimentally observed dripline. The repulsive effects of filling the $d_{3/2}$ is also observed in ^{29}F . However, the inclusion of an extra proton provides enough extra binding to keep the latter isotope bound by about 700 keV with respect to ^{25}F , in much better agreement with the experimental value of 1.47 MeV. The induced interaction alone would overestimate this binding and pre-existing 3NFs are fundamental in achieving the correct balancing between the attraction generated by the extra proton and the repulsion due to the filling of the neutron sd shell.

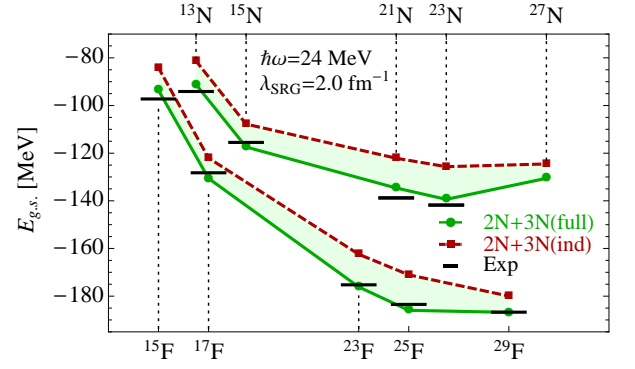


FIG. 4. (Color online) Binding energies of odd-even nitrogen and fluorine isotopes calculated for induced (red squares) and full (green dots) interactions. Experimental data are from [33].

In conclusion, we have considered the extension of the SCGF method to include three-body hamiltonians. By properly defining system dependent effective one- and two-body interactions that include the relevant contribution from 3NFs, calculations can be performed with formalisms already existing for two-body Hamiltonians. This approach, however, goes beyond usual truncations based on normal ordering of the Hamiltonian and employs fully correlated densities instead of unperturbed reference states. We applied this approach for the first time to study SRG-evolved chiral 2N and 3N interactions on the isotopic chains of nitrogen, oxygen and fluorine. We find that chiral 3NF at N2LO are crucial in predicting the binding energies of these isotopes and they reproduce the correct behaviour at the neutron driplines for all three cases. Within the estimated errors due to the many-body techniques and the dependence on the SRG evolutions, we find a remarkable agreement between our calculations and the experimental energies along all three isotopic chains.

Recent results [11] clearly show that state of the art SCGF methods can be straightforwardly extended to the corresponding Gorkov formalism for open shells, which is now underway. This would not only allows direct calculations of semi-magic even-even isotopes with analogous quality as above but would also allow extracting a wealth of information on neigh-

bor isotopes reachable by transfer of one or two nucleons.

Acknowledgements. This work was supported by the United Kingdom Science and Technology Facilities Council (STFC) under Grant ST/J000051/1 and the Natural Sciences and Engineering Research Council of Canada (NSERC) Grant No. 401945-2011. TRIUMF receives funding via a contribution through the National Research Council Canada.

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